

Universal corrections to scaling for block entanglement in spin- $\frac{1}{2}$ XX chains

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Abstract. We consider the Rényi entropies $S_n(\ell)$ in the one dimensional spin-1/2 Heisenberg XX chain in a magnetic field. The case $n = 1$ corresponds to the von Neumann “entanglement” entropy. Using a combination of methods based on the generalized Fisher-Hartwig conjecture and a recurrence relation connected to the Painlevé VI differential equation we obtain the asymptotic behaviour, accurate to order $\mathcal{O}(\ell^{-3})$, of the Rényi entropies $S_n(\ell)$ for large block lengths ℓ . For $n = 1, 2, 3, 10$ this constitutes the 3, 6, 10, 48 leading terms respectively. The $o(1)$ contributions are found to exhibit a rich structure of oscillatory behaviour, which we analyze in some detail both for finite n and in the limit $n \rightarrow \infty$.

1. Introduction

Let $|\Psi\rangle$ be the ground state of an extended quantum mechanical system and $\rho = |\Psi\rangle\langle\Psi|$ its density matrix. In order to quantify the bipartite entanglement in the ground state one divides the Hilbert space into a part \mathcal{A} and its complement \mathcal{B} and considers the reduced density matrix $\rho_{\mathcal{A}} = \text{Tr}_{\mathcal{B}} \rho$ of subsystem \mathcal{A} . A measure of the quantum entanglement in the ground-state is provided by the Rényi entropies [1]

$$S_n = \frac{1}{1-n} \ln \text{Tr} \rho_{\mathcal{A}}^n. \quad (1)$$

The particular case $n = 1$ of (1) is known as the von Neumann entropy S_1 and it is usually called simply *entanglement entropy*. However, the knowledge of S_n for different n characterizes the full spectrum of non-zero eigenvalues of $\rho_{\mathcal{A}}$ (see e.g. [2]) and provides significantly more information on the entanglement than the more widely studied von Neumann entropy.

Of particular interest is the universal scaling behaviour exhibited by S_n at quantum critical points. For a one-dimensional critical system whose scaling limit is described by a conformal field theory (CFT) of central charge c and \mathcal{A} being an interval of length ℓ embedded in an infinite system, the asymptotic large- ℓ behaviour of the Rényi entropies is given by [3, 4, 5]

$$S_n(\ell) \simeq \frac{c}{6} \left(1 + \frac{1}{n}\right) \ln \ell + c'_n. \quad (2)$$

Here c'_n is a non-universal constant. The scaling behaviour (2) has been verified both analytically and numerically for a variety of quantum spin chains whose scaling limits are described by CFTs, see e.g. [6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17] as well as in direct field theory calculations [18]. In one dimensional systems these entanglement entropies provide a very useful way for determining the central charge c that characterizes the behaviour at conformally invariant critical points. While other methods for determining c such as the finite-size scaling of the ground state energy [19, 20] require the knowledge of certain non-universal properties such as the velocity of sound, the large- ℓ behaviour of the entanglement provides a *direct* measure of c as is apparent from Eqn (2). For this reason a scaling analysis of S_n is increasingly used in numerical studies of quantum phase transitions in one dimensional systems [21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33].

In such applications $S_n(\ell)$ is computed numerically and the large- ℓ behaviour is then fitted to the form (2). It has been observed that the asymptotic result is sometimes obscured by large, and often oscillatory, corrections to scaling [34, 35, 24, 25]. In Ref. [35], on the basis of both exact and numerical results, it has been argued that these corrections are in fact *universal* and encode information about the underlying CFT beyond what is captured by the central charge alone. More precisely, they give access to the scaling dimensions of some of the most relevant operators in the underlying CFT. This conjecture of Ref. [35] has been recently confirmed by using perturbed CFT arguments [36].

A precise characterization of the subleading terms in $S_n(\ell)$ is then desirable for two reasons. First, the knowledge of their structure will be helpful when using (2) to extract the central charge from numerical computations of $S_n(\ell)$. Second, the subleading terms can be used to infer the scaling dimensions of certain operators in the CFT characterising the quantum critical point. This motivates the present

study, in which we significantly extend our recent calculation [35] of the subleading corrections to the Rényi entropies in the XX chain.

1.1. Spin-1/2 XX Chain

The Hamiltonian of the XX model on an infinite one dimensional chain is

$$H = - \sum_{l=-\infty}^{\infty} \frac{1}{2} [\sigma_l^x \sigma_{l+1}^x + \sigma_l^y \sigma_{l+1}^y] - h \sigma_l^z, \quad (3)$$

where $\sigma_l^{x,y,z}$ are the Pauli matrices at site l . The Jordan-Wigner transformation

$$c_l = \left(\prod_{m<l} \sigma_m^z \right) \frac{\sigma_l^x + i \sigma_l^y}{2}, \quad (4)$$

maps this model to a quadratic Hamiltonian of spinless fermions

$$H = - \sum_{l=-\infty}^{\infty} c_l^\dagger c_{l+1} + c_{l+1}^\dagger c_l + 2h \left(c_l^\dagger c_l - \frac{1}{2} \right). \quad (5)$$

Here h represents the chemical potential for the spinless fermions c_l , which satisfy canonical anti-commutation relations $\{c_l, c_m^\dagger\} = \delta_{l,m}$. The Hamiltonian (5) is diagonal in momentum space and for $|h| < 1$ the ground-state is a partially filled Fermi sea with Fermi-momentum

$$k_F = \arccos |h|. \quad (6)$$

In the following we will always assume that $|h| < 1$ so that we are dealing with a gapless theory.

1.2. Entanglement Entropy of the XX chain: Jin-Korepin Result

A key result regarding on entanglement measures in the XX chain is due to Jin and Korepin [8], who obtained the leading large- ℓ behaviour of S_n . Their result takes the form

$$S_n^{JK}(\ell) = \frac{1}{6} \left(1 + \frac{1}{n} \right) \ln(2\ell |\sin k_F|) + E_n, \quad (7)$$

where the constant E_n has the integral representation

$$E_n = \left(1 + \frac{1}{n} \right) \int_0^\infty \frac{dt}{t} \left[\frac{1}{1 - n^{-2}} \left(\frac{1}{n \sinh t/n} - \frac{1}{\sinh t} \right) \frac{1}{\sinh t} - \frac{e^{-2t}}{6} \right]. \quad (8)$$

The objective of our work is to determine the subleading corrections to $S_n^{JK}(\ell)$ for large, finite block lengths ℓ . It is therefore convenient to introduce quantities $d_n(\ell)$

$$d_n(\ell) \equiv S_n(\ell) - S_n^{JK}(\ell), \quad (9)$$

to which we will refer throughout.

The remainder of this paper is organized as follows. For the sake of clarity we first present a summary of our results in section 2. When then turn to the details of our derivations. In section 3 we briefly review one of our key tools, the *generalized Fisher-Hartwig conjecture*. The latter is used in section 4 to determine all “harmonic” corrections to the Rényi entanglement entropies. In order to go beyond the generalized Fisher Hartwig conjecture we utilize recent developments related to

Random Matrix Theory. These are introduced in section 5 and used to determine “non-harmonic” terms in the asymptotic expansion for the von Neumann and Rényi entropies in sections 6 and 7 respectively. Comparisons between our analytic expansion and numerical results are presented in section 8.

2. Summary of Results

This section contains a summary of our results.

2.1. Rényi Entropies of the XX chain: General Result

Our full result for $d_n(\ell)$ can be cast in the form

$$d_n(\ell) = \frac{2}{n-1} \sum_{p,q=1}^{\infty} (-1)^p L_k^{-\frac{2p(2q-1)}{n}} (Q_{n,q})^p \left[\frac{\cos(2k_F \ell p)}{p} + \frac{A_q \sin(2k_F p \ell)}{L_k} + \frac{[B_{p,q}^{(n)} e^{2ipk_F \ell} + \text{h.c.}]}{L_k^2} \right] + \frac{1}{L_k^2} \frac{n+1}{285n^3} (15(3n^2-7) + (49-n^2) \sin^2 k_F) + \mathcal{O}(L_k^{-3}), \quad (10)$$

where

$$L_k = 2\ell |\sin k_F|, \quad (11)$$

$$A_q = \left[1 + 3 \left(\frac{2q-1}{n} \right)^2 \right] \cos k_F, \quad (12)$$

$$Q_{n,q} = \left[\frac{\Gamma(\frac{1}{2} + \frac{2q-1}{2n})}{\Gamma(\frac{1}{2} - \frac{2q-1}{2n})} \right]^2, \quad (13)$$

$$B_{p,q}^{(n)} = \frac{2q-1}{6n} \left[\left(5 + 7 \frac{(2q-1)^2}{n^2} \right) \sin^2(k_F) - 15 \left(\frac{(2q-1)^2}{n^2} + 1 \right) \right] - \frac{p}{4} \left[\left(1 + 3 \frac{(2q-1)^2}{n^2} \right) \cos(k_F) \right]^2. \quad (14)$$

The leading contribution to $d_n(\ell)$ has already been announced in Ref. [35] and is given by

$$d_n(\ell) = \frac{2 \cos(2k_F \ell)}{1-n} (2\ell |\sin k_F|)^{-2/n} Q_{n,1} + \mathcal{O}(\ell^{-\min[4/n, 2]}). \quad (15)$$

2.2. Rényi Entropies of the XX chain: explicit results for $S_2(\ell)$ and $S_3(\ell)$

In the special cases $n=2$ and $n=3$ our results read

$$d_2(\ell) = -\frac{2Q_{2,1} \cos(2k_F \ell)}{L_k} + \frac{1}{L_k^2} \left[Q_{2,1}^2 \cos(4k_F \ell) - \frac{7Q_{2,1} \cos k_F}{2} \sin(2k_F \ell) + \frac{5+3 \sin^2 k_F}{64} \right] + \mathcal{O}(L_k^{-3}), \quad (16)$$

and

$$\begin{aligned}
 d_3(\ell) = & -\frac{Q_{3,1} \cos(2k_F \ell)}{L_k^{2/3}} + \frac{Q_{3,1}^2 \cos(4k_F \ell)}{2L_k^{4/3}} - \frac{4Q_{3,1} \cos k_F \sin(2k_F \ell)}{3L_k^{5/3}} \\
 & - \frac{Q_{3,1}^3 \cos(6k_F \ell)}{3L_k^2} + 2\frac{15 + 2\sin^2 k_F}{243L_k^2} + \frac{4 \cos(k_F) Q_{3,1}^2 \sin(4k_F \ell)}{3L_k^{7/3}} \\
 & + \frac{Q_{3,1}^4 \cos(8k_F \ell)}{4L_k^{8/3}} + \frac{2Q_{3,1}(111 - 62\sin^2(k_F)) \cos(2k_F \ell)}{81L_k^{8/3}} + \mathcal{O}(L_k^{-3}). \quad (17)
 \end{aligned}$$

2.3. Rényi Entropies of the XX chain: limit $n \rightarrow \infty$

In the limit $n \rightarrow \infty$ infinitely many terms in (10) combine to generate a logarithmic contribution, whose general expression is is given in Eq. (70). It assumes a particularly simple form at half-filling $k_F = \pi/2$

$$d_\infty(\ell) \simeq \frac{\pi^2}{24 \ln(2b\ell)} \begin{cases} 2 & \ell \text{ odd} , \\ -1 & \ell \text{ even} , \end{cases} \quad (18)$$

where $b = \exp(-\Psi(1/2)) \approx 7.12429$.

2.4. von Neumann Entropy of the XX chain

In the special case $n = 1$ corresponding to the von Neumann entropy all oscillating contributions to (10) vanish. This explains why it is easier to determine the central charge from S_1 than from Rényi entropies with $n \geq 2$ (this is no longer true in the presence of boundaries [34], where it is found that oscillations persist in the limit $n \rightarrow 1$). Specializing Eq. (10) to $n = 1$ we obtain

$$S_1 \simeq \frac{1}{3} \ln \ell + c'_1 - \frac{1}{12\ell^2} \left(\frac{1}{5} + \cot k_F^2 \right). \quad (19)$$

In this expression, the ℓ^{-2} power-law behaviour is *universal* [35, 13].

3. Entanglement entropy in the XX model

Let us return to the spin-1/2 XX model on an infinitely long chain (3). The reduced density matrix of a block of ℓ contiguous sites can be expressed as

$$\rho_A = \det C \exp \left(\sum_{j,l \in A} [\ln(C^{-1} - 1)]_{jl} c_j^\dagger c_l \right), \quad (20)$$

where the *correlation matrix* C has matrix elements

$$C_{nm} = \langle c_m^\dagger c_n \rangle = \frac{\sin k_F(m-n)}{\pi(m-n)}. \quad (21)$$

As a real symmetric matrix C can be diagonalized by a unitary transformation

$$UCU^\dagger \equiv \delta_{lm}(1 + \nu_m)/2. \quad (22)$$

This implies that the reduced density matrix ρ_ℓ is uncorrelated in the transformed basis. The Rényi entropies can be expressed in terms of the eigenvalues ν_l as

$$S_n(\ell) = \sum_{l=1}^{\ell} e_n(\nu_l), \quad \text{with} \quad e_n(x) = \frac{1}{1-n} \ln \left[\left(\frac{1+x}{2} \right)^n + \left(\frac{1-x}{2} \right)^n \right]. \quad (23)$$

More details about this procedure can be found in e.g. Refs. [6, 16, 37]. We note that the above construction refers to the block entanglement of fermionic degrees of freedom. However, in the case considered here, the non-locality induced by the Jordan-Wigner transformation does not affect the reduced density matrix. In fact, it can be seen to mix only spins inside the block. This ceases to be the case when two or more disjoint intervals are considered [38, 39] and other techniques need to be employed [40] in order to recover CFT predictions [41, 42, 38].

The representation (23) is particularly convenient for numerical computations: the eigenvalues ν_m of the $\ell \times \ell$ correlation matrix C are determined by standard linear algebra methods and $S_n(\ell)$ is then computed using Eq. (23). In order to obtain the universal behaviour in the limit of large block lengths $\ell \rightarrow \infty$ we follow Ref. [8]. We introduce the determinant

$$D_\ell(\lambda) = \det((\lambda + 1)I - 2C) \equiv \det(G). \quad (24)$$

In the eigenbasis of C the determinant is simply a polynomial of degree ℓ in λ with zeroes $\{\nu_j | j = 1, \dots, \ell\}$, i.e.

$$D_\ell(\lambda) = \prod_{j=1}^{\ell} (\lambda - \nu_j). \quad (25)$$

This implies that the Rényi entropies have the integral representation

$$S_n(\ell) = \frac{1}{2\pi i} \oint d\lambda \, e_n(\lambda) \frac{d \ln D_\ell(\lambda)}{d\lambda}, \quad (26)$$

where the contour of integration encircles the segment $[-1, 1]$. The matrix G is a $\ell \times \ell$ Toeplitz matrix, i.e. its matrix elements depend only on the difference between row and column indices

$$G_{jk} = g_{j-k}. \quad (27)$$

In the theory of Toeplitz matrices an important role is played by the Fourier transform $g(\theta)$ of g_l

$$g_l = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{il\theta} g(\theta). \quad (28)$$

The function $g(\theta)$ is called *symbol* and in our case takes the form

$$g(\theta) = \begin{cases} \lambda + 1 & \theta \in [k_F, 2\pi - k_F] \\ \lambda - 1 & \theta \in [0, k_F] \cup [2\pi - k_F, 2\pi] \end{cases}. \quad (29)$$

On the interval $[0, 2\pi]$ the function $g(\theta)$ has two discontinuities at $\theta_1 = k_F$ and $\theta_2 = 2\pi - k_F$.

3.1. The generalized Fisher-Hartwig conjecture

The Fisher-Hartwig conjecture [43] gives the asymptotic behaviour of the determinant of a Toeplitz matrix in the limit where the dimension ℓ of the matrix becomes large. This has been used by Jin and Korepin [8] to derive the leading large ℓ asymptotic behaviour of the Rényi entanglement entropies. As stressed in Ref. [8], for the Toeplitz matrices defined by the symbol (29) the Fisher-Hartwig conjecture has been proven by Basor [44].

In order to employ the Fisher-Hartwig conjecture one needs to express the symbol $g(\theta)$ of a Toeplitz matrix in the form

$$g(\theta) = f(\theta) \prod_{r=1}^R e^{ib_r[\theta - \theta_r - \pi \text{sgn}(\theta - \theta_r)]} (2 - 2 \cos(\theta - \theta_r))^{a_r}, \quad (30)$$

where R is an integer, a_r , b_r and θ_r are constants and $f(\theta)$ is a smooth function with winding number zero. The Fisher-Hartwig conjecture then states that the large- ℓ asymptotic behaviour of the corresponding Toeplitz determinant is given by

$$D_\ell \sim F[f(\theta)]^\ell \left(\prod_{j=1}^R \ell^{a_j^2 - b_j^2} \right) E, \quad (31)$$

where $F[f(\theta)] = \exp(\frac{1}{2\pi} \int_0^{2\pi} d\theta \ln f(\theta))$ and E is a known function of $f(\theta)$, a_r , b_r , and θ_r . In our case it is straightforward to express the symbol in the canonical form (30). As $g(\theta)$ has two discontinuities in $[0, 2\pi)$ we have $R = 2$. It is useful to define a function

$$\beta_\lambda = \frac{1}{2\pi i} \ln \left[\frac{\lambda + 1}{\lambda - 1} \right], \quad (32)$$

where the branch cut of the logarithm is chosen such that

$$-\pi \leq \arg \left[\frac{\lambda + 1}{\lambda - 1} \right] < \pi. \quad (33)$$

Inserting the ansatz

$$b_1 = -b_2, \quad a_{1,2} = 0, \quad f(\theta) = f_0 = \text{const} \quad (34)$$

into (30) gives

$$g(\theta) = f_0 e^{2ib_2 k_F} \begin{cases} 1 & \theta \in [k_F, 2\pi - k_F] \\ e^{-2\pi i b_2} & \theta \in [0, k_F] \cup [2\pi - k_F, 2\pi] \end{cases}. \quad (35)$$

Comparing (35) to (29) we conclude that we require

$$b_2 = \beta_\lambda + m, \quad (36)$$

where m is an arbitrary integer number. We further identify

$$f_0 = (\lambda + 1) e^{-2ib_2 k_F} = (\lambda + 1) e^{-2ik_F m} e^{-2ik_F \beta_\lambda}. \quad (37)$$

The integer m labels the different inequivalent *representations* of the symbol $g(\theta)$, see [44]. In their work Jin and Korepin employed the Fisher-Hartwig conjecture for the $m = 0$ representation and obtained the following result for the large- ℓ asymptotics of $D_\ell(\lambda)$ [8]

$$D_\ell^{JK}(\lambda) \sim \left[(\lambda + 1) \left(\frac{\lambda + 1}{\lambda - 1} \right)^{-\frac{k_F}{\pi}} \right]^\ell L_k^{-2\beta^2(\lambda)} G^2(1 + \beta_\lambda) G^2(1 - \beta_\lambda), \quad (38)$$

where $L_k = 2\ell |\sin k_F|$ has been introduced in (11). Inserting (38) into (26) and carrying out the integral leads to the result for the asymptotic behaviour of the Rényi entropy reported in Eq. (7). Expression (7) provides the leading behaviour of $S_n(\ell)$ for large block lengths ℓ . It is the purpose of our work to determine (universal) subleading contributions to (7). This is achieved by noting that for the case when the symbol $g(\theta)$ has several inequivalent representations labelled by an integer m the asymptotics

of the corresponding Toeplitz determinant is given by the so-called *generalized Fisher-Hartwig conjecture* (gFHC) [44], which reads

$$D_\ell(\lambda) \sim \sum_m e^{l_0^{(m)}\ell - \sum_{r=1}^2 (b_r^{(m)})^2} E^{(m)}. \quad (39)$$

In our case, the various parameters in (39) are given by

$$l_0^{(m)} = \ln(f_0^{(m)}) = \ln(\lambda + 1) - 2ik_F\beta_\lambda - 2ik_Fm, \quad (40)$$

$$b_2^{(m)} = -b_1^{(m)} = \beta_\lambda + m, \quad (41)$$

where m are integers and

$$E^{(m)} = [2 - 2\cos(2k_F)]^{-(\beta_\lambda + m)^2} [G(1 + \beta_\lambda + m)G(1 - \beta_\lambda - m)]^2. \quad (42)$$

Here $G(z)$ is the Barnes G -function [45]. We note that the gFHC has been used to determine the large-distance asymptotics of various two-point correlation functions in Refs [46, 47]. Important properties of the gFHC in our case are

- (i) The exponential increase is representation independent and governed by the exponent

$$\text{Re}(l_0^{(m)}) = \text{Re}[\ln(\lambda + 1)] - \frac{k_F}{\pi} \text{Re} \left[\ln \left[\frac{\lambda + 1}{\lambda - 1} \right] \right] \quad (43)$$

- (ii) The leading oscillatory behaviour depends on the representation and is given by

$$\text{Im}(l_0^{(m)}) = \text{Im}[\ln(\lambda + 1)] - \frac{k_F}{\pi} \text{Im} \left[\ln \left[\frac{\lambda + 1}{\lambda - 1} \right] \right] - 2k_Fm. \quad (44)$$

- (iii) The power law correction depends on the representation and is characterized by the exponents

$$\alpha_m = (b_1^{(m)})^2 + (b_2^{(m)})^2 = -2(\beta_\lambda + m)^2. \quad (45)$$

The real parts of these exponents are

$$\text{Re}(\alpha_m) = -2\text{Re}(\beta_\lambda^2) - 2m(m + 2\text{Re}(\beta_\lambda)). \quad (46)$$

In conjunction with the inequality $-1 \leq 2\text{Re}(\beta_\lambda) < 1$ this establishes that

$$\text{Re}(\alpha_m) \leq \text{Re}(\alpha_0). \quad (47)$$

Equality in (47) holds only for $m = 1$ and $\text{Re}(\beta_\lambda) = -\frac{1}{2}$, which corresponds to the case $-1 < \lambda < 1$.

We note that point (iii) is crucial for Eqn (38) to give the correct asymptotic behaviour of $S_n(\ell)$: along the integration contour in (26) we always have $\text{Im}(\lambda) \neq 0$. Representations with $m \neq 0$ therefore give subleading corrections, which we are going to analyze in the following section.

The full result of the generalized Fisher-Hartwig conjecture for the Toeplitz determinant takes the form

$$D_\ell \sim (\lambda + 1)^\ell \left(\frac{\lambda + 1}{\lambda - 1} \right)^{-\frac{k_F\ell}{\pi}} \sum_{m \in \mathbb{Z}} L_k^{-2(m+\beta_\lambda)^2} e^{-2ik_Fm\ell} \times [G(m + 1 + \beta_\lambda)G(1 - m - \beta_\lambda)]^2. \quad (48)$$

4. Corrections to the scaling for entanglement

The leading corrections to scaling for the Rényi entropies are obtained from the “harmonic” terms given by the generalized Fisher-Hartwig conjecture. It follows from (46) that the most important corrections arise from the first two contributions with $m = \pm 1$. Keeping only the three terms corresponding to $m = -1, 0, 1$ in (48) we obtain the following expression for the asymptotics of the determinant $D_\ell(\lambda)$

$$D_\ell \sim D_\ell^{JK} \left[1 + e^{-2ik_F \ell} L_k^{-2-4\beta_\lambda} \frac{G^2(2+\beta_\lambda)G^2(-\beta_\lambda)}{G^2(1+\beta_\lambda)G^2(1-\beta_\lambda)} + e^{2ik_F \ell} L_k^{-2+4\beta_\lambda} \frac{G^2(2-\beta_\lambda)G^2(\beta_\lambda)}{G^2(1+\beta_\lambda)G^2(1-\beta_\lambda)} \right]. \quad (49)$$

Here $D_N^{JK}(\lambda)$ is given in Eq. (38). Using $G(1+x)/G(x) = \Gamma(x)$ we can rewrite the last formula as

$$D_\ell(\lambda) \sim D_\ell^{JK} (1 + \Psi_\ell(\lambda)) , \quad \Psi_\ell(\lambda) = e^{-2ik_F \ell} L_k^{-2(1+2\beta_\lambda)} \frac{\Gamma^2(1+\beta_\lambda)}{\Gamma^2(-\beta_\lambda)} + e^{2ik_F \ell} L_k^{-2(1-2\beta_\lambda)} \frac{\Gamma^2(1-\beta_\lambda)}{\Gamma^2(\beta_\lambda)}. \quad (50)$$

It follows from the factorized form of (50) that the contributions of the correction terms to the entropies are easier to calculate than the contribution of the leading term D_ℓ^{JK} itself. This will enable us to obtain a full analytic answer. For large L_k we have (we recall that $d_n(\ell) = S_n(\ell) - S_n^{JK}(\ell)$)

$$d_n(\ell) \sim \frac{1}{2\pi i} \oint d\lambda e_n(\lambda) \frac{d \ln [1 + \Psi_\ell(\lambda)]}{d\lambda} = \frac{1}{2\pi i} \oint d\lambda e_n(\lambda) \frac{d\Psi_\ell(\lambda)}{d\lambda} + \dots \quad (51)$$

The contour integral can be written as the sum of two contributions infinitesimally above and below the interval $[-1, 1]$ respectively, i.e.

$$d_n(\ell) \sim \frac{1}{2\pi i} \left[\int_{-1+i\epsilon}^{1+i\epsilon} - \int_{-1-i\epsilon}^{1-i\epsilon} \right] d\lambda e_n(\lambda) \frac{d\Psi_\ell(\lambda)}{d\lambda}. \quad (52)$$

This shows that we only require the discontinuity across the branch cut. The only discontinuous function is β_λ , which for $-1 < x < 1$ behaves as

$$\beta_{x \pm i\epsilon} = -iw(x) \mp \frac{1}{2}, \quad \text{with} \quad w(x) = \frac{1}{2\pi} \ln \frac{1+x}{1-x}. \quad (53)$$

We now change variables from λ to w

$$\lambda = \tanh(\pi w), \quad -\infty < w < \infty. \quad (54)$$

We have

$$\begin{aligned} \left[L_k^{-2-4\beta} \frac{\Gamma^2(1+\beta)}{\Gamma^2(-\beta)} \right]_{\beta=-iw-\frac{1}{2}} - \left[L_k^{-2-4\beta} \frac{\Gamma^2(1+\beta)}{\Gamma^2(-\beta)} \right]_{\beta=-iw+\frac{1}{2}} &\simeq L_k^{4iw} \gamma^2(w), \\ \left[L_k^{-2+4\beta} \frac{\Gamma^2(1-\beta)}{\Gamma^2(\beta)} \right]_{\beta=-iw-\frac{1}{2}} - \left[L_k^{-2+4\beta} \frac{\Gamma^2(1-\beta)}{\Gamma^2(\beta)} \right]_{\beta=-iw+\frac{1}{2}} &\simeq -L_k^{-4iw} \gamma^2(-w), \end{aligned}$$

where we have dropped terms of order $O(L_k^{-4})$ compared to the leading ones and we have defined

$$\gamma(w) = \frac{\Gamma(\frac{1}{2} - iw)}{\Gamma(\frac{1}{2} + iw)}. \quad (55)$$

Integrating by parts and using

$$\frac{d}{dw} e_n(\tanh(\pi w)) = \frac{\pi n}{1-n} (\tanh(n\pi w) - \tanh(\pi w)), \quad (56)$$

we arrive at

$$d_n(\ell) \sim \frac{in}{2(1-n)} \int_{-\infty}^{\infty} dw (\tanh(\pi w) - \tanh(n\pi w)) \times \\ \times [e^{-2ik_F\ell} L_k^{4iw} \gamma^2(w) - e^{2ik_F\ell} L_k^{-4iw} \gamma^2(-w)] + \dots \quad (57)$$

For large ℓ the leading contribution to the integral arises from the poles closest to the real axis. These are located at $w_0 = i/2n$ ($w_0 = -i/2n$) for the first (second) term in (57). Evaluating their contributions to the integral gives

$$d_n(\ell) = \frac{2 \cos(2k_F\ell)}{1-n} (2\ell |\sin k_F|)^{-2/n} \left[\frac{\Gamma(\frac{1}{2} + \frac{1}{2n})}{\Gamma(\frac{1}{2} - \frac{1}{2n})} \right]^2 + o(\ell^{-2/n}). \quad (58)$$

This result implies that at half-filling ($k_F = \frac{\pi}{2}$) and $n > 1$ the corrections are positive (negative) for odd (even) ℓ .

4.1. Subleading Corrections

Eqn (58) describes the asymptotic behaviour in the limit $L_k \rightarrow \infty$, n fixed. It provides a good approximation for large, finite ℓ as long as $\ln(L_k) \gg n$. This is a strong restriction already for moderate values of n . For example, L_k is required to be larger than 10^4 for $n = 10$. For practical purposes it is useful to know the corrections to $S_n(\ell)$ for large ℓ but $\ln(L_k)$ not necessarily much larger than n . In this regime there are two main sources of corrections to (58).

- (i) The integral (56) is no longer dominated by the poles closest to the real axis and contributions from further poles need to be included. These give rise to corrections proportional to $L_k^{-2q/n}$, with q integer.
- (ii) Further terms in the expansion of the logarithm in Eqn (51) need to be taken into account. The corresponding contributions are proportional to $e^{\pm i2pk_F\ell}$ with $p = 2, 3, \dots$

At half-filling (zero magnetic field) the situation is different in that terms with odd p all give rise to an overall factor $(-1)^\ell$ and hence modify the staggered contribution to $S_n(\ell)$, while terms with even p add to the smooth (non-oscillatory) part already present in $S_n^{JK}(\ell)$.

We now take both types of corrections into account. We first consider the series expansion of the logarithm in Eq. (51)

$$\ln [1 + \Psi_\ell(\lambda)] = \sum_{p=1}^{\infty} \frac{(-1)^{p+1} (\Psi_\ell(\lambda))^p}{p}. \quad (59)$$

Recalling the explicit expression (50) for $\Psi_\ell(\lambda)$ leads to a binomial sum

$$(\Psi_\ell(\lambda))^p = \left(e^{-2ik_F\ell} L_k^{-2(1+2\beta_\lambda)} c_{\beta_\lambda} + e^{2ik_F\ell} L_k^{-2(1-2\beta_\lambda)} c_{-\beta_\lambda} \right)^p \\ = \sum_{q=0}^p \binom{p}{q} e^{2ik_F\ell(2q-p)} L_k^{-2p} L_k^{-4(p-2q)\beta_\lambda} c_{\beta_\lambda}^{p-q} c_{-\beta_\lambda}^q, \quad (60)$$

where we have introduced the shorthand notation $c_\beta = (\Gamma(1 + \beta)/\Gamma(-\beta))^2$. When calculating the discontinuity across the branch cut running from $\lambda = -1$ to $\lambda = 1$ all terms other than $q = 0$ and $q = p$ give rise to terms that are subleading in L_k . Hence we may approximate

$$\begin{aligned} (\Psi_\ell(\tanh(\pi w) + i\epsilon))^p - (\Psi_\ell(\tanh(\pi w) - i\epsilon))^p &\approx e^{-2ik_F\ell p} L_k^{4iwp} c_{-iw-1/2}^p \\ &+ e^{2ik_F\ell p} L_k^{-4iwp} c_{-iw+1/2}^p. \end{aligned} \quad (61)$$

The analog of (57) then reads

$$\begin{aligned} d_n(\ell) &\sim \sum_{p=1}^{\infty} \frac{(-1)^{p+1}}{p} \frac{in}{2(1-n)} \int_{-\infty}^{\infty} dw (\tanh(\pi w) - \tanh(n\pi w)) \\ &\times \left[e^{-2ipk_F\ell} L_k^{4iwp} \gamma^{2p}(w) - e^{2ipk_F\ell} L_k^{-4iwp} \gamma^{2p}(-w) \right]. \end{aligned} \quad (62)$$

The integral is carried out by contour integration, taking the two terms in square brackets into account separately. The first (second) contribution has simple poles in the upper (lower) half plane at $w_q = i\frac{2q-1}{2n}$ ($w_q = -i\frac{2q-1}{2n}$), where q is a positive integer such that $2q-1 \neq n, 3n, 5n, \dots$. Contour integration then gives

$$d_n(\ell) = \frac{2}{1-n} \sum_{p,q=1}^{\infty} \frac{(-1)^{p+1}}{p} \cos(2k_F\ell p) L_k^{-\frac{2p(2q-1)}{n}} (Q_{n,q})^p + \mathcal{O}(L_k^{-1-2/n}), \quad (63)$$

where the constants $Q_{n,q}$ have been defined in (13). In the sum over q the special values $2q-1 \neq n, 3n, 5n, \dots$ are to be omitted. In particular, this means that for $n = 1$ all these corrections are absent. Eqn (63) is one of the main results of our work. It shows that there are contributions to the Rényi entropies with oscillation frequencies that are arbitrary multiples of $2k_F$.

At half-filling ($k_F = \pi/2$) certain simplifications occur. For even ℓ we find

$$d_n(\ell) \sim \frac{2}{1-n} \left[(2\ell)^{-\frac{2}{n}} Q_{n,1} - (2\ell)^{-\frac{4}{n}} \frac{Q_{n,1}^2}{2} + (2\ell)^{-\frac{6}{n}} \left(\frac{Q_{n,1}^3}{3} + Q_{n,3} \right) \right] + \dots, \quad (64)$$

while for odd ℓ we obtain

$$d_n(\ell) \sim \frac{-2}{1-n} \left[(2\ell)^{-\frac{2}{n}} Q_{n,1} + (2\ell)^{-\frac{4}{n}} \frac{Q_{n,1}^2}{2} + (2\ell)^{-\frac{6}{n}} \left(\frac{Q_{n,1}^3}{3} + Q_{n,3} \right) \right] + \dots \quad (65)$$

In all the above analysis we have ignored contributions to the generalized Fisher-Hartwig conjecture with $|m| > 1$. While these lead to oscillatory contributions with frequencies that are integer multiples of $2k_F$ they are suppressed by additional powers of ℓ^{-1} and hence are subleading, even in the case where n is not small.

It is apparent from (63) that the limit $n \rightarrow \infty$ deserves special attention. $S_\infty(\ell)$ is known in the literature as *single copy entanglement* [48]. Here it is necessary to sum up an infinite number of contributions in order to extract the large- ℓ asymptotics. We note that the large- n limit is not only of academic interest, but will provide information on the behaviour of $S_n(\ell)$ in the regime $n \gg \ln L_k$, $L_k \gg 1$.

4.2. Large n limit of $S_n(\ell)$

In order to investigate the limit $n \rightarrow \infty$ we consider eqn (62), but now first take the parameter n to infinity and then carry out the resulting integrals. This gives

$$d_\infty(\ell) \sim \frac{i}{2} \sum_{p=1}^{\infty} \frac{(-1)^p}{p} \int_{-\infty}^{\infty} dw (\text{sgn}(w) - \tanh(\pi w))$$

$$\begin{aligned}
 & \times \left[e^{-2ik_F \ell p} L_k^{4iwp} [\gamma(w)]^{2p} e^{2ik_F \ell p} L_k^{-4iwp} [\gamma(-w)]^{2p} \right] \\
 &= - \sum_{p=1}^{\infty} \frac{(-1)^p}{p} \left[e^{-2ik_F \ell p} \text{Im} \int_0^{\infty} dw [1 - \tanh(\pi w)] L_k^{4iwp} [\gamma(w)]^{2p} \right. \\
 & \quad \left. - e^{2ik_F \ell p} \text{Im} \int_0^{\infty} dw [1 - \tanh(\pi w)] L_k^{-4iwp} [\gamma(-w)]^{2p} \right]. \quad (66)
 \end{aligned}$$

Using that the first singularity in the upper (lower) half plane occurs at $w = i/2$ ($w = -i/2$) we deform the contours to run parallel to the real axis with imaginary parts $i/4$ and $-i/4$ respectively, i.e. for the first term we use

$$\int_0^{\infty} dw f(w) = \int_0^{i/4} dw f(w) + \int_{i/4}^{\infty+i/4} dw f(w).$$

It is straightforward to show that the second integral contributes only to order $O(1/L_k)$ and does not give rise to logarithmic corrections. Hence the leading contribution is of the form

$$\begin{aligned}
 d_{\infty}(\ell) &\sim \sum_{p=1}^{\infty} \frac{(-1)^p}{p} \left[e^{-2ik_F \ell p} \text{Re} \int_0^{1/4} dz (1 - i \tan(\pi z)) L_k^{-4zp} (\gamma(iz))^{2p} \right. \\
 & \quad \left. + e^{2ik_F \ell p} \text{Re} \int_0^{1/4} dz (1 + i \tan(\pi z)) L_k^{-4zp} (\gamma(iz))^{2p} \right] \\
 &= 2 \sum_{p=1}^{\infty} \frac{(-1)^p}{p} \cos(2k_F \ell p) \int_0^{1/4} dz e^{-4zp \ln L_k} (\gamma(iz))^{2p}. \quad (67)
 \end{aligned}$$

For large L_k the dominant contribution to integral is obtained by expanding $(\gamma(iz))^{2p}$ in a power series around $z = 0$

$$\begin{aligned}
 d_{\infty}(\ell) &\sim 2 \sum_{p=1}^{\infty} \frac{(-1)^p}{p} \cos(2k_F \ell p) \int_0^{1/4} dz e^{-4zp \ln L_k} (1 + 4pz \Psi(1/2) + \dots) \\
 &= 2 \sum_{p=1}^{\infty} \frac{(-1)^p}{p^2} \cos(2k_F \ell p) \left[\frac{1}{4 \ln L_k} + \frac{\Psi(1/2)}{4 \ln^2 L_k} + \dots \right] + O(L_k^{-1}), \quad (68)
 \end{aligned}$$

where $\Psi(x)$ is the digamma function. The leading contribution can be expressed in terms of the dilogarithm function $\text{Li}_2(x)$ using

$$2 \sum_{p=1}^{\infty} \frac{(-1)^p}{p^2} \cos(2k_F \ell p) = \text{Li}_2(-e^{i2k_F \ell}) + \text{Li}_2(-e^{-i2k_F \ell}). \quad (69)$$

In the half-filled case ($k_F = \pi/2$) our result takes a particularly simple form

$$d_{\infty}(\ell) \sim \frac{1}{2 \ln L_k} \sum_{p=1}^{\infty} \frac{(-1)^{p(\ell+1)}}{p^2} = \begin{cases} \frac{1}{2 \ln L_k} \frac{\pi^2}{6} & \ell \text{ odd} , \\ -\frac{1}{2 \ln L_k} \frac{\pi^2}{12} & \ell \text{ even} . \end{cases} \quad (70)$$

Summing some of the subleading terms in (68) to all orders in $(\ln(L_k))^{-1}$ leads to an expression of the form

$$d_{\infty}(\ell) \sim \frac{\pi^2}{24 \ln(bL_k)} \begin{cases} 2 & \ell \text{ odd} , \\ -1 & \ell \text{ even} , \end{cases} \quad (71)$$

where $b = \exp(-\Psi(1/2)) \approx 7.12429$. This is found to be in good agreement with numerical computations.

5. Connection with random matrix theory

Keating and Mezzadri [49] have shown that the Toeplitz determinant $D_\ell(\lambda)$ is related to an important quantity in random matrix theory, namely the gap probability for the circular unitary ensemble (CUE). The generating function $E_\ell^{\text{CUE}}[(0, \phi); \xi]$ (in the following we will drop all arguments to ease notations) for the probability of finding exactly k eigenvalues $e^{i\theta}$ within the segment $\theta \in (\pi - \phi, \pi]$ of the unit circle is given by [50]

$$E_\ell^{\text{CUE}} \equiv \frac{1}{(2\pi)^\ell \ell!} \left(\int_{-\pi}^{\pi} -\xi \int_{\pi-\phi}^{\pi} \right) d\theta_1 \dots \left(\int_{-\pi}^{\pi} -\xi \int_{\pi-\phi}^{\pi} \right) d\theta_\ell \prod_{1 \leq j < k \leq \ell} |e^{i\theta_j} - e^{i\theta_k}|^2.$$

This is equal to the determinant of the Toeplitz matrix [50]

$$W_{ij} = w_{i-j}, \quad \text{with } w_n = \delta_{n,0} + \frac{\xi}{2\pi i} (-1)^{n+1} \frac{e^{in\phi} - 1}{n}. \quad (72)$$

It then follows that for $\xi = 2/(\lambda + 1)$ and $\phi = 2k_F$ we have [49]

$$D_\ell(\lambda) = (\lambda + 1)^\ell E_\ell^{\text{CUE}}. \quad (73)$$

For any value of ℓ the generating function E_ℓ^{CUE} can be determined from a recurrence relations connected to the Painlevé VI transcendent [50]. The recurrence relation reads

$$x_\ell x_{\ell-1} - c = \frac{1 - x_\ell^2}{2x_\ell} [(\ell + 1)x_{\ell+1} + (\ell - 1)x_{\ell-1}] - \frac{1 - x_{\ell-1}^2}{2x_{\ell-1}} [\ell x_\ell + (\ell - 2)x_{\ell-2}], \quad (74)$$

where $c = \cos k_F$ and the initial values are

$$x_{-1} = 0, \quad x_0 = 1, \quad x_1 = -\frac{\xi}{\pi} \frac{\sin k_F}{1 - \frac{\xi}{\pi} k_F}. \quad (75)$$

The generating function is related to x_ℓ by

$$\frac{E_{\ell+1}^{\text{CUE}} E_{\ell-1}^{\text{CUE}}}{(E_\ell^{\text{CUE}})^2} = 1 - x_\ell^2 = \frac{D_{\ell+1} D_{\ell-1}}{D_\ell^2}. \quad (76)$$

For the sake of completeness we quote the values of the generating function for $\ell = 0$ and $\ell = 1$

$$E_0^{\text{CUE}} = 1, \quad E_1^{\text{CUE}} = 1 - \frac{\xi}{2\pi} \phi. \quad (77)$$

5.1. Leading large- ℓ asymptotics of x_ℓ

In Ref. [49] it was suggested to combine the asymptotic results (38) following from the Fisher-Hartwig conjecture with the recurrence relation (74) in order to obtain further corrections to the large- ℓ behaviour of the Rényi entropies. Inserting (38) into (76) suggests that [49]

$$x_\ell = \frac{\sqrt{2}|\beta_\lambda|}{\ell} + O(\ell^{-2}). \quad (78)$$

However, a numerical solution of the recurrence relation shows that (78) does not generally provide the correct large- ℓ asymptotics of x_ℓ . The reason for this is as follows. When we substitute the “full” result (50) of the *generalized* Fisher-Hartwig conjecture into (74) we find that the contributions due to the representations with $m = \pm 1$ behave as $\ell^{-1 \pm 2\beta_\lambda}$ for large ℓ . For any $\text{Re}(\beta_\lambda) \neq 0$ one of these will dominate over the contribution arising from the $m = 0$ term that gives rise to Eq. (78). In other words *subleading* contributions to $D_\ell(\lambda)$ give rise to the *leading* large- ℓ behaviour of x_ℓ !

We now show in more detail how to extract the large- ℓ behaviour of x_ℓ from that of $D_\ell(\lambda)$. In order to keep things simple, we focus on the case $\text{Re}(\beta_\lambda) > 0$. Here we may neglect the terms with $|m| > 1$ and $m = -1$ in (48), which leads to

$$\frac{D_{\ell+1}D_{\ell-1}}{D_\ell^2} \sim \left[1 + \frac{2\beta_\lambda^2}{\ell^2}\right] (1 - 4a_0^2 e^{2ik_F\ell} \ell^{-2+4\beta_\lambda} \sin^2 k_F) + \dots, \quad (79)$$

where we have introduced

$$a_0 = (2 \sin k_F)^{-1+2\beta_\lambda} \frac{\Gamma(1-\beta_\lambda)}{\Gamma(\beta_\lambda)}. \quad (80)$$

The contribution in square brackets arises from the $m = 0$ Fisher-Hartwig term and is the result quoted in Ref. [49]. For $\text{Re}(\beta_\lambda) > 0$ this term is subleading and we obtain instead

$$x_\ell \sim (-1)^\ell e^{ik_F\ell} \ell^{-1+2\beta_\lambda} (2 \sin k_F)^{2\beta_\lambda} \frac{\Gamma(1-\beta_\lambda)}{\Gamma(\beta_\lambda)}, \quad \text{Re}(\beta_\lambda) > 0. \quad (81)$$

Here we have fixed the sign of x_ℓ by requiring that the expression (81) asymptotically satisfies the recurrence relation (74). The analogous analysis in the case $\text{Re}(\beta_\lambda) < 0$ gives

$$x_\ell \sim (-1)^\ell e^{-ik_F\ell} \ell^{-1-2\beta_\lambda} (2 \sin k_F)^{-2\beta_\lambda} \frac{\Gamma(1+\beta_\lambda)}{\Gamma(-\beta_\lambda)}, \quad \text{Re}(\beta_\lambda) < 0. \quad (82)$$

We may combine Eqns (81) and (82) into a single equation

$$x_\ell \sim \frac{(-1)^\ell}{\ell} \left[e^{ik_F\ell} (2\ell \sin k_F)^{2\beta_\lambda} \frac{\Gamma(1-\beta_\lambda)}{\Gamma(\beta_\lambda)} + e^{-ik_F\ell} (2\ell \sin k_F)^{-2\beta_\lambda} \frac{\Gamma(1+\beta_\lambda)}{\Gamma(-\beta_\lambda)} \right] + \dots \quad (83)$$

We emphasize that (83) must not be understood as giving the two leading terms in the large- ℓ asymptotic expansion of x_ℓ because e.g. for $\text{Re}(\beta_\lambda) > \frac{1}{6}$ there are other contributions to x_ℓ that decay more slowly than $\ell^{-1-2\beta_\lambda}$. In order to check the result (83) we have solved the recurrence relation (74) numerically for a number of different values of λ and k_F . In Fig. 1 we compare the asymptotic expression (83) against the numerically computed values for x_ℓ . The agreement is seen to be excellent in all cases.

5.2. Asymptotic expansion for x_ℓ and analytic corrections to the gFHC expression for $D_\ell(\lambda)$

We now turn to the derivation of contributions to the large- ℓ asymptotic expansion for $D_\ell(\lambda)$ that are not contained in the gFHC. This will be achieved by utilizing the recurrence relation (74).

We expect the asymptotics of $D_\ell(\lambda)$ to be such that each harmonic term predicted by gFHC is multiplied by a function analytic in $1/\ell$. Restricting our attention to the

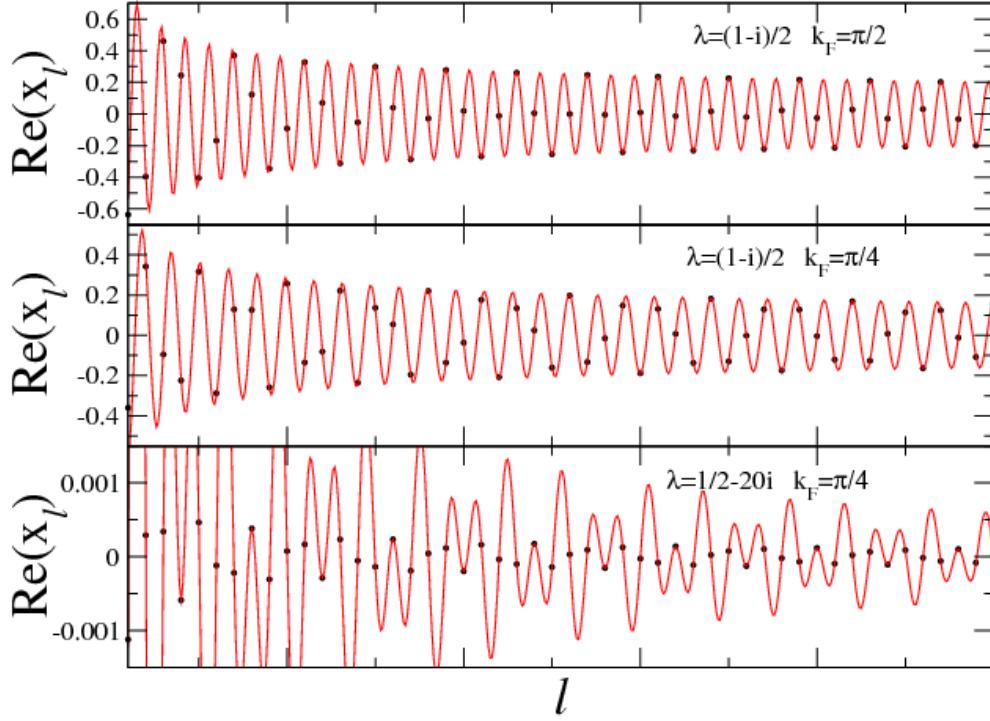


Figure 1. Real part of x_ℓ as a function of ℓ for several values of λ and k_F . The points are obtained from a numerical solution of the recurrence relation (74). The continuous lines are obtained from the asymptotic prediction (83) by the replacement $(-1)^\ell \rightarrow e^{i\pi\ell}$. The first two panels correspond to the same value $\beta_\lambda \simeq 0.323792 - 0.128075i$ but two different values of k_F . The last panel corresponds to $\beta_\lambda \sim 0.0158924 - 0.0003966i$ and hence the contributions of both terms in Eq. (83) are important. In all cases we observe good agreement of the theoretical prediction (83) with the numerical data.

first three harmonic terms (i.e. $m = -1, 0, 1$), this leads to an expansion of the form

$$\begin{aligned} \frac{D_\ell}{D_\ell^{JK}} \sim & \left[1 + \frac{c_1}{\ell} + \frac{c_2}{\ell^2} + \dots \right] + a_0^2 e^{2ik_F\ell} \ell^{-2(1-2\beta_\lambda)} \left[1 + \frac{a_1}{\ell} + \frac{a_2}{\ell^2} + \dots \right] \\ & + b_0^2 e^{-2ik_F\ell} \ell^{-2(1+2\beta_\lambda)} \left[1 + \frac{b_1}{\ell} + \frac{b_2}{\ell^2} + \dots \right], \end{aligned} \quad (84)$$

where a_0 is given by (80) and

$$b_0 = (2 \sin k_F)^{-1-2\beta_\lambda} \frac{\Gamma(1+\beta_\lambda)}{\Gamma(-\beta_\lambda)}. \quad (85)$$

We note that by definition we have

$$(2 \sin k_F)^2 a_0 b_0 = -\beta_\lambda^2. \quad (86)$$

We now proceed in a straightforward albeit extremely tedious way:

- (i) We first insert (84) into (76) in order to obtain an expression for the asymptotic expansion for x_ℓ .

- (ii) We input the resulting expression into the recurrence relation (74) for x_ℓ and determine the parameters characterizing the asymptotic expansion of x_ℓ order by order in ℓ^{-1} .

The result of step (i) for $\text{Re}(\beta_\lambda) > 0$ is

$$\begin{aligned} \frac{x_\ell}{x_\ell^{\text{asy}}} &= \sum_{j=0}^3 (-1)^j \left[1 + \frac{o_{j1}}{\ell} + \frac{o_{j2}}{\ell^2} + \frac{o_{j3}}{\ell^3} + \dots \right] a_0^{2j} e^{2ik_F j \ell} \ell^{j(-2+4\beta_\lambda)} \\ &+ \sum_{j=1}^2 \frac{\ell^{-4j\beta_\lambda} e^{-2ik_F j \ell}}{(2a_0 \sin k_F)^{2j}} \left[q_{j0} + \frac{q_{j1}}{\ell} + \frac{q_{j2}}{\ell^2} + \dots \right] + \dots, \end{aligned} \quad (87)$$

where we have written only the terms required for our purposes and where we have introduced the quantity

$$x_\ell^{\text{asy}} = (-1)^\ell e^{ik_F \ell} \ell^{-1+2\beta_\lambda} 2a_0 \sin k_F. \quad (88)$$

The explicit expressions for the coefficients o_{jl} and q_{jl} in terms of the expansion coefficients a_j, b_j , and c_j characterizing the large- ℓ asymptotics of D_ℓ are reported in Appendix A.

Step (ii) consists of substituting (87) in the recurrence relation (74) and determining the coefficients o_{jl} and q_{jl} . The non-linearity of (74) renders this a very difficult task, because terms at different orders in ℓ^{-1} in x_ℓ contribute to the same order in the recurrence relation. For this reason it is crucial to retain sufficiently many terms in (87). The results of this procedure are reported in Appendix B.

Combining the results reported in Appendix A and Appendix B then yields the desired expressions for the expansion coefficients a_j, b_j and c_j

$$\begin{aligned} c_1(\beta_\lambda) &= 2\beta_\lambda^3 i \cot k_F, \\ c_2(\beta_\lambda) &= \frac{\beta_\lambda^2}{6} (-1 + 7\beta_\lambda^2 + 12\beta_\lambda^4 - 3\beta_\lambda^2(5 + 4\beta_\lambda^2) \csc^2 k_F), \\ b_j(\beta_\lambda) &= c_j(\beta_\lambda + 1), \quad j = 1, 2, \\ a_j(\beta_\lambda) &= c_j(\beta_\lambda - 1), \quad j = 1, 2. \end{aligned} \quad (89)$$

6. Corrections to the von Neumann entropy

Having determined the asymptotic expansion for $D_\ell(\lambda)$ we may now use (26) to calculate additional subleading contributions to the Rényi entropies. We first consider the von Neumann entropy (the case $n = 1$), in which as we have seen above all harmonic contributions vanish. Taking the limit $n \rightarrow 1$ in (26) and following through the same steps as in section 4 we find

$$d_1(\ell) \sim \frac{i}{2} \int_{-\infty}^{\infty} dw \frac{\pi w}{\cosh^2 \pi w} \left[\frac{c_1^+ - c_1^-}{\ell} + \frac{2c_2^+ - (c_1^+)^2 - 2c_2^- + (c_1^-)^2}{2\ell^2} \right], \quad (90)$$

where we have defined

$$c_j^\pm = c_j(-iw \mp \frac{1}{2}), \quad j = 1, 2. \quad (91)$$

Here $c_{1,2}$ are given by (89) and we have used

$$\lim_{n \rightarrow 1} \frac{\tanh(\pi w) - \tanh(n\pi w)}{1 - n} = \frac{\pi w}{\cosh^2 \pi w}. \quad (92)$$

As $c_1^+ - c_1^-$ is an even function of w the $\mathcal{O}(\ell^{-1})$ contribution in (90) vanishes. The $\mathcal{O}(\ell^{-2})$ contribution can be calculate analytically using the integrals

$$\int_{-\infty}^{\infty} dw \frac{\pi w^2}{\cosh^2 \pi w} = \frac{1}{6}, \quad \int_{-\infty}^{\infty} dw \frac{\pi w^4}{\cosh^2 \pi w} = \frac{7}{120}, \quad (93)$$

which gives the final result

$$d_1(\ell) \sim -\frac{1}{12\ell^2} \left[\frac{1}{5} + \cot^2 k_F \right]. \quad (94)$$

The simplicity of this answer suggests the existence of a much more straightforward derivation than ours.

7. Corrections to the Rényi entropies

The case of the Rényi entropies is more complicated because the contribution of the harmonic terms does not vanish. Our starting point is the expansion (84) for the Toeplitz determinant, which we express in the form

$$\frac{D_\ell}{D_\ell^{JK}} \sim 1 + \Psi_\ell(\beta_\lambda) + \frac{\delta\Psi_\ell^{(1)}(\beta_\lambda)}{\ell} + \frac{\delta\Psi_\ell^{(2)}(\beta_\lambda)}{\ell^2} + \dots \quad (95)$$

Here $\Psi_\ell(\beta_\lambda)$ are the contributions we have taken into account previously in section 4. The logarithm of the Toeplitz determinant is expanded as

$$\begin{aligned} \ln \left[\frac{D_\ell}{D_\ell^{JK}} \right] &\sim \ln \left[1 + \Psi_\ell(\beta_\lambda) + \frac{\delta\Psi_\ell^{(1)}(\beta_\lambda)}{\ell} + \frac{\delta\Psi_\ell^{(2)}(\beta_\lambda)}{\ell^2} \right] \\ &\approx \sum_{p=1}^{\infty} \frac{(-1)^{p+1}}{p} \left\{ [\Psi_\ell(\beta_\lambda)]^p + p \frac{\delta\Psi_\ell^{(1)}(\beta_\lambda) [\Psi_\ell(\beta_\lambda)]^{p-1}}{\ell} \right. \\ &\quad \left. + p \frac{[\Psi_\ell(\beta_\lambda)]^{p-1} \delta\Psi_\ell^{(2)}(\beta_\lambda) + \frac{p-1}{2} [\delta\Psi_\ell^{(1)}(\beta_\lambda)]^2 [\Psi_\ell(\beta_\lambda)]^{p-2}}{\ell^2} \right\} \\ &\equiv \chi^{(0)}(\beta_\lambda) + \frac{\chi^{(1)}(\beta_\lambda)}{\ell} + \frac{\chi^{(2)}(\beta_\lambda)}{\ell^2}. \end{aligned} \quad (96)$$

Following through the same steps as in section 4 we then arrive at the following expansion for the Rényi entropies

$$\begin{aligned} d_n(\ell) &\sim \frac{in}{2(1-n)} \int_{-\infty}^{\infty} dw (\tanh(\pi w) - \tanh(n\pi w)) \\ &\quad \times \left[\chi^{(0)}(\beta_\lambda) + \frac{\chi^{(1)}(\beta_\lambda)}{\ell} + \frac{\chi^{(2)}(\beta_\lambda)}{\ell^2} \right]_{\beta_\lambda = -iw - \frac{1}{2}}^{\beta_\lambda = -iw + \frac{1}{2}} \\ &= d_n^{(0)}(\ell) + d_n^{(1)}(\ell) + d_n^{(2)}(\ell). \end{aligned} \quad (97)$$

The contribution $d_n^{(0)}(\ell)$ has been determined in section 4. The other two contributions are calculated by the same method as in section 4 and we find

$$d_n^{(1)}(\ell) \sim \frac{2 \cos(k_F)}{1-n} \sum_{p,q=1}^{\infty} (-1)^{p+1} \sin(2k_F p \ell) L_k^{-1 - \frac{2p(2q-1)}{n}}$$

$$\times \left[1 + 3 \left(\frac{2q-1}{n} \right)^2 \right] \left[\frac{\Gamma\left(\frac{1}{2} + \frac{2q-1}{2n}\right)}{\Gamma\left(\frac{1}{2} - \frac{2q-1}{2n}\right)} \right]^{2p}, \quad (98)$$

$$d_n^{(2)}(\ell) \sim \frac{2}{n-1} \sum_{p,q=1}^{\infty} (-1)^p L_k^{-2-\frac{2p(2q-1)}{n}} \left[\frac{\Gamma\left(\frac{1}{2} + \frac{2q-1}{2n}\right)}{\Gamma\left(\frac{1}{2} - \frac{2q-1}{2n}\right)} \right]^{2p} \left[B_{p,q}^{(n)} e^{2ipk_F \ell} + \text{h.c.} \right] \\ + \frac{1}{\ell^2} \frac{n+1}{1440n^3} \left(49 - n^2 + \frac{15(3n^2-7)}{\sin^2 k_F} \right). \quad (99)$$

Explicit expressions for the coefficients $B_{pq}^{(n)}$ are given in Appendix C.

8. Numerical results

Given our asymptotic expansion a natural question to ask is how well it approximates the Rényi entropies for large but finite block lengths ℓ . In order to address this question we will now present a number of comparisons between our asymptotic result and numerically exact expressions for $S_n(\ell)$. The latter are obtained by determining the eigenvalues of the Toeplitz matrix C_{nm} in Eq. (21) and computing S_n from Eq. (23).

8.1. Leading contributions to $d_n(\ell)$

In the top two panels of Fig.2 we plot the absolute value of $d_n(\ell)$ for $n = 2$ and $n = \infty$ at $k_F = \pi/2$ and compare it to the leading asymptotic expressions (15) and (71) respectively. We see that the asymptotic expressions give good agreement with the numerically exact results even for moderate values of ℓ .

The next issue we turn to is the behaviour of $S_n(\ell)$ for large, finite values of n . In this case the asymptotic power-law $d_n(\ell) \propto \ell^{-2/n}$ only emerges for very large block lengths $\ln \ell \gg n$. On the other hand, for smaller values of ℓ the numerical data is seen to follow the large n prediction (71) as is shown in the bottom panel of Fig. 2. Here we plot $1/|d_n(\ell)|$, which at large values of ℓ will grow as $\ell^{2/n}$. A logarithmic behaviour for small small values of ℓ is clearly visible, which then crosses over to the expected $\ell^{2/n}$ regime at approximately $\ln \ell \sim n$. It appears that the crossover scale is larger for even ℓ . We expect a crossover between these two regimes to be a generic feature in critical theories. This suggests that in such gapless models particular care is required when studying $S_n(\ell)$ for large n .

8.2. Corrections to the von Neumann entropy $S_1(\ell)$

For the von Neumann entropy S_1 all the oscillating terms vanish and the predicted large- ℓ asymptotic behaviour is given in Eq. (19). In Fig.3 we plot $-\ell^2 d_1(\ell)$ as a function of ℓ and compare it with the prediction (19). We see that the agreement is excellent, which indicates that further corrections are very small. We note that for vanishing magnetic field ($k_F = \pi/2$) the amplitude of the $\mathcal{O}(\ell^{-2})$ correction term is numerically small (1/60) so that the corresponding contribution to $S_1(\ell)$ becomes negligible already for relatively small ℓ . At least in the particular case of the XX model in zero field this shows that the central charge is most conveniently extracted from finite-size scaling studies of $S_1(\ell)$ rather than higher Rényi entropies.

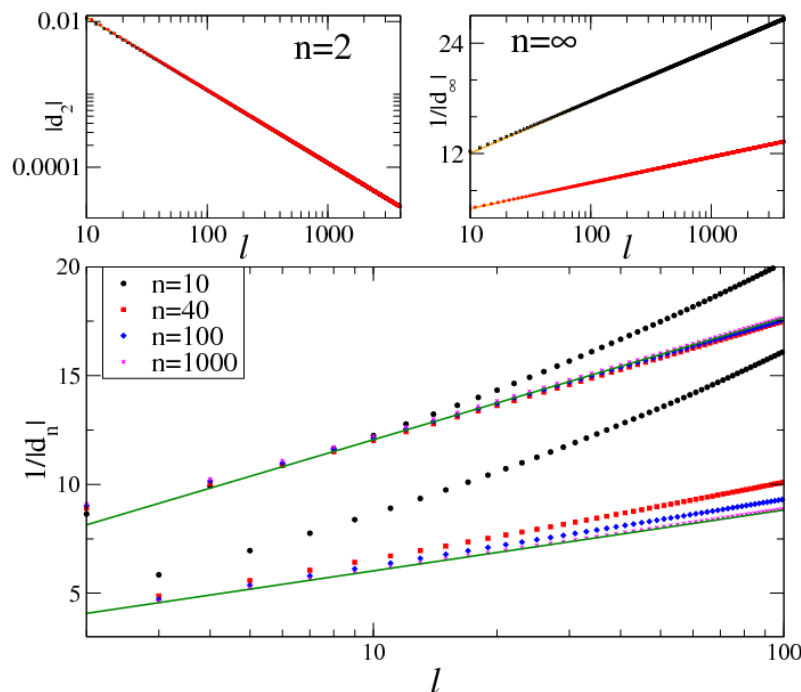


Figure 2. Top: $d_n(\ell) = S_n(\ell) - S_n^{JK}(\ell)$ at half-filling ($k_F = \frac{\pi}{2}$) for $n = 2$ and $n = \infty$ compared to the asymptotic expressions (straight lines for even/odd ℓ respectively). The agreement is seen to be excellent even for moderate values of ℓ . Bottom: $|d_n(\ell)|^{-1}$ as a function of ℓ for several values of n and $k_F = \frac{\pi}{2}$. The straight lines show the asymptotic results (71) in the limit $n \rightarrow \infty$ for even and odd ℓ respectively. We see that for large n the correction $d_n(\ell)$ exhibits a logarithmic increase up to a block size $\ln \ell \sim n$, when the asymptotic behaviour starts to be seen (as we are plotting $|d_n(\ell)|^{-1}$ the asymptotic behaviour corresponds to a $\ell^{2/n}$ power-law increase with ℓ).

8.3. Subleading contributions to $d_n(\ell)$

For $n > 1$ the structure subleading corrections to scaling for $S_n(\ell)$ is significantly richer. Explicit expressions, accurate to order $O(\ell^{-3})$, for the cases $n = 2$ and $n = 3$ are given in Eqns (16) and (17) respectively. A comparison of these results for $n = 2$ to numerical computations is presented in Fig.4. We have chosen $k_F = \pi/4$ so as to be able to separate the oscillation frequencies of the various contributions. The top panel in Fig. 4 presents a comparison of the asymptotic expression for $d_2(\ell)$ (continuous lines) to numerical computations (dots) and show good agreement even for small ℓ . In order to better assess the accuracy of the asymptotic results we introduce the rescaled, subtracted quantity

$$D_2(\ell) = [d_2(\ell) - d_2^{\text{asy}}(\ell)]\ell^2, \quad (100)$$

where $d_2^{\text{asy}}(\ell)$ represents the leading correction given in Eq. (15). By construction $D_2(\ell)$ should tend to a sum of oscillatory terms with fixed amplitudes for large ℓ . The four-sublattice oscillatory behaviour of $D_2(\ell)$ predicted by (16) is clearly visible and as expected we observe excellent agreement between the numerical and asymptotic results. For larger values of n , the corrections arising from the ‘analytic’ part of $D_\ell(\lambda)$

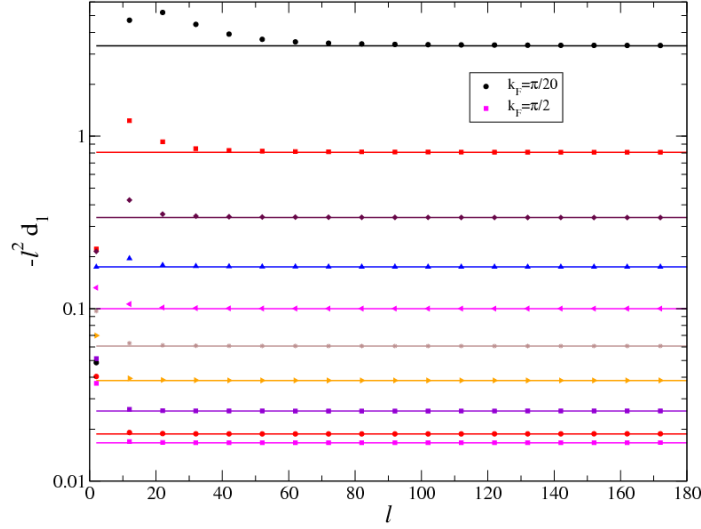


Figure 3. Correction to scaling for the von Neumann entropy $d_1 = S_1 - S_1^{JK}$. We plot the quantity $-\ell^2 d_1(\ell)$ for values $k_F = n\pi/20$, where $n = 1$ (top curve) up to $n = 10$ (bottom curve). The straight lines are our prediction Eq. (19).

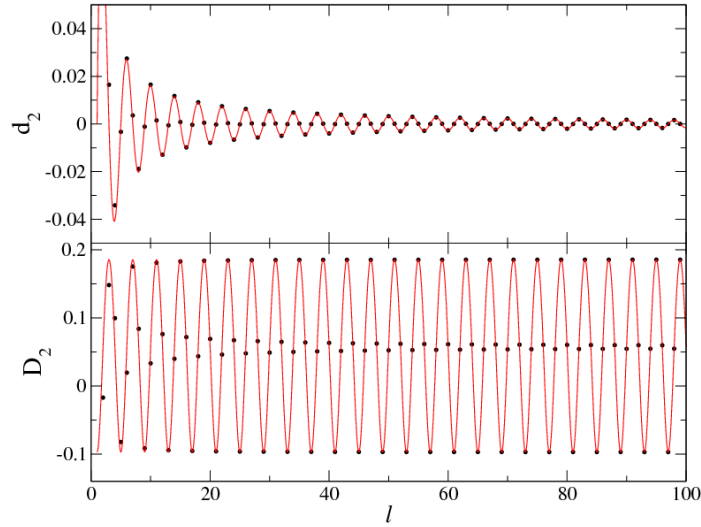


Figure 4. Corrections to scaling for the Rényi entropy $S_2(\ell)$ at $k_F = \pi/4$. Upper panel: $d_2(\ell)$ as a function of ℓ . Dots are the numerical results while the continuous line corresponds to the asymptotic expression (16). Lower panel: rescaled subleading corrections $D_2(\ell)$ defined in (100) as a function of ℓ . The agreement between the asymptotic expression (continuous line) and numerical data (dots) confirms that (16) is correct to order $o(\ell^{-2})$.

are less important than the harmonic contributions. Thus the most relevant terms in the asymptotic expansion are those given in Eq. (63). In fact, the first analytic correction has an exponent $-1-2/n$ and at a given n appears only after $[n/2]$ harmonic

contributions with exponents $-2p/n$ with $p = 1, 2, \dots$. It has already been observed in Ref. [35] that for higher values of n the first subleading order does not suffice to give an accurate description of the Rényi entropies.

In Fig. 5 we show a comparison of the corrections $d_n(\ell)$ for $n = 10, 20$ and $k_F = \pi/4$ with the asymptotic result Eq. (63). Step by step we take into account further terms in the asymptotic expression (63) until we obtain good agreement with the numerical data. We observe that for $n = 10$ three terms in Eq. (63) are enough to reproduce the data, while for $n = 20$ we need five terms to have the same accuracy.

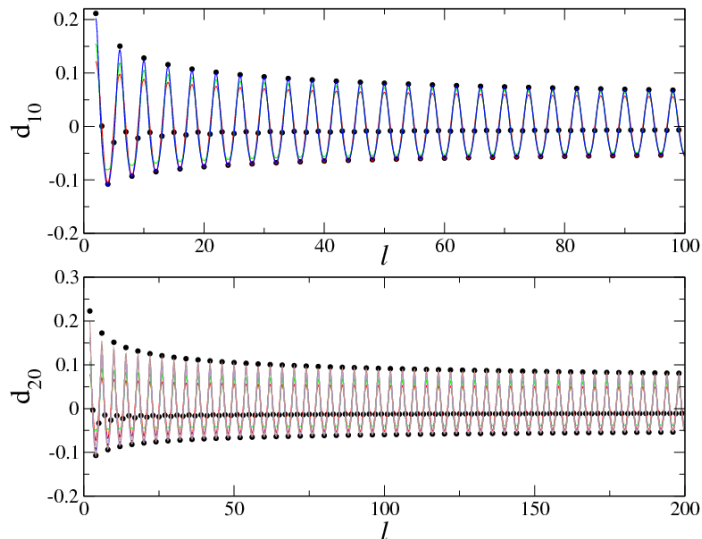


Figure 5. Corrections $d_n(\ell)$ for $n = 10$ (top) and $n = 20$ (bottom) for $k_F = \pi/4$. The numerical data are well described by Eq. (63), but more terms are needed to obtain the same degree of accuracy when n is increased. In both plots the various continuous curves correspond to Eq. (63) one (red curve), two (green curve), three (blue curve), etc terms in (63) retained.

9. Conclusions

In this work we have determined the asymptotic behaviour of the Rényi entropies $S_n(\ell)$ in the spin-1/2 XX model for large block lengths ℓ . A summary of our results has been presented in section 2. While we have considered the specific case of the spin-1/2 XX chain in a magnetic field, some features we find are in fact universal. In particular, the scaling of the leading oscillatory term (15) has been observed for the XXZ model in zero magnetic field in Ref. [35]. The corresponding exponent is modified to $\ell^{-2K/n}$, where K the Luttinger liquid parameter. This is in full agreement with recent perturbed CFT calculations [36]. As we have emphasized repeatedly, a precise knowledge of the structure of the oscillating terms in $S_n(\ell)$ is useful for extracting properties such as the central charge and scaling dimensions of certain operators at quantum critical points. They furthermore can be used for analyzing numerical studies of more complicated quantities such as the entanglement of two disjoint intervals [38, 40].

Oscillating behaviour has also been observed in numerical studies of other entanglement estimators [51] such as the valence-bond entanglement. A natural

question is whether these can be determined for certain models using the free fermion techniques we employed for the XX case as well.

Finally we would like to remark that our results carry over directly to the critical Ising chain. According to Ref. [12], the R nyi entropies in the critical Ising model (with $c = 1/2$) are related to those of the spin-1/2 XX chain in zero magnetic field ($k_F = \pi/2$) by

$$S_n^{\text{Is}}(\ell) = \frac{1}{2} S_n^{\text{XX}}(2\ell, k_F = \pi/2). \quad (101)$$

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Appendix A. Relation between the expansion coefficients for D_ℓ and x_ℓ

In this appendix we report the relations between the coefficients a_i , b_i and c_i in the asymptotic expansion (84) of the Toeplitz determinant $D_\ell(\lambda)$ and the expansion coefficients o_{jl} , q_{jl} characterizing the large- ℓ behaviour (87) of the auxiliary quantities x_ℓ . The following relations hold:

$$\begin{aligned} o_{j1} &= i(1 - 2\beta_\lambda) \cot k_F + \frac{a_1 - c_1}{2}(2j + 1), \\ o_{j2} &= (j + \frac{1}{2})(a_2 - c_2) + (1 - 3\beta_\lambda + 3\beta_\lambda^2) + i \cot k_F(2j + 1 - (j + 1)\beta)(a_1 - c_1) \\ &\quad + \frac{2j + 1}{8}(a_1 - c_1)((2j - 1)a_1 - (2j + 3)c_1) - \delta_{j0} \left[\frac{1 - \beta_\lambda}{2 \sin k_F} \right]^2, \\ q_{10} &= -\beta_\lambda^2, \\ q_{11} &= \beta_\lambda^2 \left[\frac{a_1 - c_1}{2} + i(1 - 2\beta_\lambda) \cot k_F \right] - c_1, \\ q_{12} &= \frac{(a_2 - c_2)\beta_\lambda^2}{2} - 3c_2 + \frac{a_1 c_1 (\beta_\lambda^2 + 2)}{4} - \frac{3a_1^2 \beta_\lambda^2}{8} + \frac{c_1^2 (\beta_\lambda^2 + 8)}{8} - \frac{\beta_\lambda^2 (1 - 2\beta_\lambda + 5\beta_\lambda^2)}{2} \\ &\quad + ((a_1 - c_1)\beta_\lambda^3 + (1 - 2\beta_\lambda)c_1)i \cot k_F + \frac{\beta_\lambda^2 (3 - 14\beta_\lambda + 15\beta_\lambda^2)}{4 \sin^2 k_F}, \\ q_{20} &= 0, \\ q_{21} &= \beta_\lambda^4 \left(\frac{a_1 + b_1}{2} - 4\beta_\lambda i \cot k_F \right) - \beta_\lambda^2 (\beta_\lambda^2 + 1)c_1. \end{aligned} \quad (\text{A.1})$$

We have derived relations for some other coefficients such as o_{03} and o_{13} , but they are not needed for our purposes and we therefore refrain from reporting them here.

Appendix B. Expansion coefficients for x_ℓ

Substituting the expansion (87) into the recurrence relation (74) gives a set of consistency relations for the coefficients q_{jl} and o_{jl} in (87). These read

$$q_{20} = q_{30} = q_{40} = q_{21} = q_{31} = q_{41} = 0, \quad (\text{B.1})$$

$$o_{11} = 3o_{01} - 2(1 - 2\beta_\lambda)i \cot k_F, \quad (\text{B.2})$$

$$q_{11} = q_{10}(-o_{01} + 2\beta_\lambda i \cot k_F), \quad (\text{B.3})$$

$$o_{j1} = o_{01} + 2j(o_{01} - (1 - 2\beta_\lambda)i \cot k_F), \quad (\text{B.4})$$

$$o_{02} = \frac{\beta_\lambda(-1 + 12\beta_\lambda - 32\beta_\lambda^2 + 27\beta_\lambda^3)}{6} + \frac{\beta_\lambda(2 - 13\beta_\lambda + 32\beta_\lambda^2 - 18\beta_\lambda^3)}{4 \sin^2 k_F}, \quad (\text{B.5})$$

$$q_{12} = \beta_\lambda^2 o_{02} - \beta_\lambda^4(4 + 9\beta_\lambda^2) + \frac{\beta_\lambda^4}{2 \sin^2 k_F}(13 + 18\beta_\lambda^2). \quad (\text{B.6})$$

Appendix C. Expressions for the coefficients B_{pq}

We recall the expressions for the coefficients $c_{1,2}$ and $b_{1,2}$ (89)

$$\begin{aligned} c_1(\beta_\lambda) &= 2\beta_\lambda^3 i \cot k_F, \\ c_2(\beta_\lambda) &= \frac{\beta_\lambda^2}{6}(-1 + 7\beta_\lambda^2 + 12\beta_\lambda^4 - 3\beta_\lambda^2(5 + 4\beta_\lambda^2) \csc^2 k_F), \\ b_j(\beta_\lambda) &= c_j(1 + \beta_\lambda), \quad j = 1, 2. \end{aligned} \quad (\text{C.1})$$

In terms of the constants $b_{j,q}^+, c_{j,q}^+$

$$b_{j,q}^+ = b_j \left(\frac{2q-1}{2n} - \frac{1}{2} \right), \quad c_{j,q}^+ = c_j \left(\frac{2q-1}{2n} - \frac{1}{2} \right), \quad j = 1, 2. \quad (\text{C.2})$$

the coefficients B_{pq} are given by

$$B_{p,q}^{(n)} = 2 \sin^2(k_F) \left[b_{2,q}^+ - \frac{(b_{1,q}^+)^2}{2} - c_{2,q}^+ + \frac{(c_{1,q}^+)^2}{2} + \frac{p}{2}(b_{1,q}^+ - c_{1,q}^+)^2 \right]. \quad (\text{C.3})$$

If $2q-1 = n, 3n, 5n, \dots$ we instead have $B_{p,q}^{(n)} = 0$. An explicit expression is

$$\begin{aligned} B_{p,q}^{(n)} &= \frac{x}{3} [(5 + 28x^2) \sin^2(k_F) - 15(4x^2 + 1)] \\ &\quad - \frac{p}{4} [(1 + 12x^2) \cos(k_F)]^2 \Big|_{x=\frac{2q-1}{2n}}. \end{aligned} \quad (\text{C.4})$$

References

- [1] L Amico, R Fazio, A Osterloh, and V Vedral, Entanglement in many-body systems, Rev. Mod. Phys. **80**, 517 (2008); J Eisert, M Cramer, and M B Plenio, Area laws for the entanglement entropy - a review, Rev. Mod. Phys. **82**, 277 (2010); Entanglement entropy in extended systems, P Calabrese, J Cardy, and B Doyon Eds, J. Phys. A **42** 500301 (2009).
- [2] P Calabrese and A Lefevre, Entanglement spectrum in one-dimensional systems, Phys. Rev. A **78**, 032329 (2008); F. Franchini, A. R. Its, V. E. Korepin, and L. A. Takhtajan, Entanglement Spectrum for the XY Model in One Dimension, 1002.2931.
- [3] C Holzhey, F Larsen, and F Wilczek, Geometric and renormalized entropy in conformal field theory, Nucl. Phys. B **424**, 443 (1994).
- [4] P Calabrese and J Cardy, Entanglement entropy and quantum field theory, J. Stat. Mech. P06002 (2004).
- [5] P Calabrese and J Cardy, Entanglement entropy and conformal field theory, J. Phys. A **42**, 504005 (2009) and references therein.
- [6] G Vidal, J I Latorre, E Rico, and A Kitaev, Entanglement in quantum critical phenomena, Phys. Rev. Lett. **90**, 227902 (2003); J I Latorre, E Rico, and G Vidal, Ground state entanglement in quantum spin chains, Quant. Inf. Comp. **4**, 048 (2004).
- [7] I. Peschel, On the entanglement entropy for a XY spin chain, J. Stat. Mech. (2004) P12005.

- [8] B-Q Jin and V E Korepin, Quantum spin chain, Toeplitz determinants and Fisher-Hartwig conjecture, *J. Stat. Phys.* **116**, 79 (2004).
- [9] A R Its, B-Q Jin, and V E Korepin, Entanglement in XY spin chain, *J. Phys. A* **38**, 2975 (2005); F Franchini, A R Its, and V E Korepin Renyi entropy of the XY spin chain, *J. Phys. A* **41** (2008) 025302.
- [10] H-Q Zhou, T Barthel, J O Fjærestad, and U Schollwoeck, Entanglement and boundary critical phenomena, *Phys. Rev. A* **74**, 050305 (2006).
- [11] G De Chiara, S Montangero, P Calabrese, and R Fazio, Entanglement entropy dynamics in Heisenberg chains, *J. Stat. Mech.* (2006) P03001.
- [12] F Igloi and R Juhasz, Exact relationship between the entanglement entropies of XY and quantum Ising chains, *Europhys. Lett.* **81**, 57003 (2008).
- [13] B Nienhuis, M Campostrini, and P Calabrese, Entanglement, combinatorics and finite-size effects in spin-chains, *J. Stat. Mech.* (2009) P02063.
- [14] M Caraglio and F Gliozzi, Entanglement entropy and twist fields, *JHEP* 0811: 076 (2008).
- [15] V Alba, M Fagotti, and P Calabrese, Entanglement entropy of excited states, *J. Stat. Mech.* (2009) P10020.
- [16] J I Latorre and A Riera, A short review on entanglement in quantum spin systems, *J. Phys. A* **42**, 504002 (2009).
- [17] F Gliozzi and L Tagliacozzo, Entanglement entropy and the complex plane of replicas, *J. Stat. Mech.* (2010) P01002.
- [18] H. Casini and M. Huerta, A finite entanglement entropy and the c-theorem *Phys. Lett. B* 600 (2004) 142; H. Casini and M. Huerta, Entanglement and alpha entropies for a massive scalar field in two dimensions, *J. Stat. Mech.* P12012 (2005); H. Casini, C. D. Fosco, and M. Huerta, Entanglement and alpha entropies for a massive Dirac field in two dimensions, *J. Stat. Mech.* P05007 (2005); J L Cardy, O A Castro-Alvaredo, and B Doyon, Form factors of branch-point twist fields in quantum integrable models and entanglement entropy, *J. Stat. Phys.* **130** (2008) 129; O A Castro-Alvaredo and B Doyon, Bi-partite entanglement entropy in massive 1+1-dimensional quantum field theories *J. Phys. A* **42**, 504006 (2009); H. Casini and M. Huerta, Entanglement entropy in free quantum field theory *J. Phys. A* **42**, 504007 (2009); T Nishioka, S Ryu, and T Takayanagi, Holographic Entanglement Entropy: An Overview, *J. Phys. A* **42** 504008 (2009); M Headrick, Entanglement Rényi entropies in holographic theories, 1006.0047.
- [19] H. W. Blöte, J. L. Cardy, and M. P. Nightingale, Conformal invariance, the central charge, and universal finite-size amplitudes at criticality, *Phys. Rev. Lett.* **56** (1986), 742.
- [20] I. Affleck, Universal term in the free energy at a critical point and the conformal anomaly, *Phys. Rev. Lett.* **56** (1986), 746.
- [21] A Laeuchli and C Kollath, Spreading of correlations and entanglement after a quench in the one-dimensional Bose-Hubbard model, *J. Stat. Mech.* P05018, (2008).
- [22] J C Xavier, Entanglement entropy, conformal invariance and the critical behavior of the anisotropic spin-S Heisenberg chains: A DMRG study, 1002.0531.
- [23] A Feiguin, S Trebst, A W W Ludwig, M Troyer, A Kitaev, Z Wang, and M H Freedman, Interacting Anyons in Topological Quantum Liquids: The Golden Chain, *Phys. Rev. Lett.* **98**, 160409 (2007).
- [24] H F Song, S Rachel, and K Le Hur, General relation between entanglement and fluctuations in one dimension, 1002.0825.
- [25] M Campostrini and E Vicari, Scaling of bipartite entanglement in one-dimensional lattice systems, with a trapping potential, 1005.3150; M Campostrini and E Vicari, Quantum critical behavior and trap-size scaling of trapped bosons in a one-dimensional optical lattice, 1003.3334.
- [26] O Legeza, J Solyom, L Tincani, and R M Noack, Entropic analysis of quantum phase transitions from uniform to spatially inhomogeneous phases, *Phys. Rev. Lett.* **99**, 087203 (2007).
- [27] L Tagliacozzo, T R. de Oliveira, S Iblisdir, and J I Latorre, Scaling of entanglement support for Matrix Product States, *Phys. Rev. B* **78**, 024410 (2008); F Pollmann, S Mukerjee, A M Turner, and J E Moore, Theory of finite-entanglement scaling at one-dimensional quantum critical points, *Phys. Rev. Lett.* **102**, 255701 (2009); N Schuch M M Wolf, F Verstraete, and J I Cirac, Entropy scaling and simulability by matrix product states, *Phys. Rev. Lett.* **100**, 030504 (2008); D Perez-Garcia, F Verstraete, M M Wolf, J I Cirac, Matrix Product State Representations *Quantum Inf. Comput.* **7**, 401 (2007).
- [28] M. Fuehringer, S. Rachel, R. Thomale, M. Greiter, and P. Schmitteckert, DMRG studies of critical SU(N) spin chains, *Ann. Phys. (Berlin)* **17**, 922 (2008).
- [29] G Roux, S Capponi, P Lecheminant, and P Azaria, Spin 3/2 fermions with attractive interactions in a one-dimensional optical lattice: phase diagrams, entanglement entropy, and the effect of

- the trap, Eur. Phys. J. B **68**, 293 (2009).
- [30] I J Cirac and G Sierra, Infinite matrix product states, conformal field theory and the Haldane-Shastry model, Phys. Rev. B **81**, 104431 (2010).
 - [31] M B Hastings, I Gonzalez, A B Kallin, R G Melko, Measuring Renyi Entanglement Entropy with Quantum Monte Carlo, 1001.2335;
 - [32] F Alet, I P. McCulloch, S Capponi, and M Mambrini, Valence bond entanglement entropy of frustrated spin chains, 1005.0787
 - [33] V Eisler and S S Garmon, Fano resonances and entanglement entropy, 1005.4612.
 - [34] N Laflorencie, E S Sorensen, M-S Chang, and I Affleck, Boundary effects in the critical scaling of entanglement entropy in 1D systems, Phys. Rev. Lett. **96**, 100603 (2006); E S Sorensen, N Laflorencie, and I Affleck, Entanglement entropy in quantum impurity systems and systems with boundaries, J. Phys. A **42**, 504009 (2009).
 - [35] P Calabrese, M Campostrini, F Essler, and B Nienhuis, Parity effects in the scaling of block entanglement in gapless spin chains, Phys. Rev. Lett. **104**, 095701 (2010).
 - [36] J Cardy and P Calabrese, Unusual Corrections to Scaling in Entanglement Entropy, J. Stat. Mech. (2010) P04023.
 - [37] I Peschel and V Eisler, Reduced density matrices and entanglement entropy in free lattice models, J. Phys. A **42**, 504003 (2009).
 - [38] V Alba, L Tagliacozzo, and P Calabrese, Entanglement entropy of two disjoint blocks in critical Ising models, Phys. Rev. B **81** (2010) 060411.
 - [39] F Igloi and I Peschel, On reduced density matrices for disjoint subsystems, 2010 EPL **89** 40001.
 - [40] M Fagotti and P Calabrese, Entanglement entropy of two disjoint blocks in XY chains, J. Stat. Mech. (2010) P04016.
 - [41] S Furukawa, V Pasquier, and J Shiraishi, Mutual information and compactification radius in a $c=1$ critical phase in one dimension, Phys. Rev. Lett. **102**, 170602 (2009).
 - [42] P Calabrese, J Cardy, and E Tonni, Entanglement entropy of two disjoint intervals in conformal field theory, J. Stat. Mech. P11001 (2009).
 - [43] M. E. Fisher and R. E. Hartwig, Toeplitz determinants: some applications, theorems, and conjectures, Adv. Chem. Phys. **15**, 333 (1968).
 - [44] E. L. Basor and C. A. Tracy, The Fisher-Hartwig conjecture and generalizations, Physica A **177**, 167 (1991); E. L. Basor and K. E. Morrison, The Fisher-Hartwig conjecture and Toeplitz eigenvalues, Linear Algebra and Its Applications **202**, 129 (1994).
 - [45] See e.g. <http://mathworld.wolfram.com/BarnesG-Function.html>.
 - [46] A.A. Ovchinnikov, Fisher-Hartwig conjecture and the correlators in XY spin chain, Phys. Lett. **A366**, 357 (2007).
 - [47] F. Franchini and A. G. Abanov, Asymptotics of Toeplitz Determinants and the Emptiness Formation Probability for the XY Spin Chain, J. Phys. A **38** (2005) 5069.
 - [48] J. Eisert and M. Cramer, Single-copy entanglement in critical spin chains, Phys. Rev. A **72**, 42112 (2005); I. Peschel and J. Zhao, On single-copy entanglement, J. Stat. Mech. P11002 (2005); R. Orus, J.I. Latorre, J. Eisert, and M. Cramer, Half the entanglement in critical systems is distillable from a single specimen, Phys. Rev. A **73**, 060303 (2006).
 - [49] J. P. Keating and F. Mezzadri, Random Matrix Theory and Entanglement in Quantum Spin Chains, Commun. Math. Phys. **252** (2004) 543; J. P. Keating and F. Mezzadri, Entanglement in Quantum Spin Chains, Symmetry Classes of Random Matrices, and Conformal Field Theory, Phys. Rev. Lett. **94** (2005) 050501.
 - [50] P.J. Forrester and N.S. Witte, Discrete Painlevé equations, Orthogonal Polynomials on the Unit Circle and N -recurrences for averages over $U(N)$ – PVI τ -functions, arXiv:math-ph/0308036; P.J. Forrester and N.S. Witte, Bi-orthogonal Polynomials on the Unit Circle, regular semi-classical Weights and Integrable Systems, Constructive Approximation **24**, 201 (2006).
 - [51] F C Alcaraz and V Rittenberg, Shared Information in Stationary States at Criticality, J. Stat. Mech. P03024 (2010); A B Kallin, I González, M B Hastings, and R Melko, Valence bond and von Neumann entanglement entropy in Heisenberg ladders, Phys. Rev. Lett. **103** (2009) 117203; F Alet, S Capponi, N Laflorencie, and M Mambrini, Valence Bond Entanglement Entropy Phys. Rev. Lett. **99**, 117204 (2007).